CROSS REFERENCE TO RELATED APPLICATIONS

This application is a divisional application of United States Application No. 08/512,815, filed August 9, 1995, now United States Patent 5,978,740.

IN THE CLAIMS

Please replace claims 19-24 with amended claims 19-24*.

19. (Amended) A method for evaluating the ability of a chemical entity to associate with a crystallized molecule or molecular complex comprising a calcineurin A (CnA) binding pocket defined by structure coordinates of CnA amino acids 90, 91, 92, 118, 120, 121, 122, 150, 151, 156, 160, 199, 232, 253, 254, 256, 281, 282, 283, 284, 306, 311, 312, and 317 according to Figure 1, or a homologue of said molecule or molecular complex wherein said homologue comprises a CnA homologue binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å;

wherein said method comprises the steps of:

* An "Appendix of Amendments" is enclosed at Tab A, showing the amendments to the claims. In the Appendix, the added portions are underscored and the deleted portions are bracketed.

B2 cont'd

a. employing computational means to perform a fitting operation between the chemical entity and the CnA binding pocket or the CnA homologue binding pocket; and

b. analyzing the results of said fitting operation to quantify the association between the chemical entity and the CnA binding pocket or the CnA homologue binding pocket.

C1 cont.

20. (Amended) The method according to claim 19, wherein said CnA binding pocket is defined by structure coordinates of CnA amino acids 90, 91, 92, 118, 120, 121, 122, 150, 151, 156, 160, 199, 281, 282, 283, 306, 311, 232, and 254, according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a CnA homologue binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

21. (Amended) A method for evaluating the ability of a chemical entity to associate with a crystallized molecule or molecular complex comprising a CnA/CnB binding pocket defined by structure coordinates of CnA amino acids 122, 124, 159, 160, 310, 312, 313, 314, 339, 341, 343, 344, 345, 347, 351, 352, 353, 354, 355, 356, 359, 360, and 363;

and calcineurin B (CnB) amino acids 49, 50, 114, 115, 118, 119, 121, 122, 123, 124, 157, 158, 159, 161, and 162 according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a CnA/CnB homologue binding pocket that has a root mean square deviation from the backbone atoms of said CnA and CnB amino acids of not more than 1.5Å;

wherein said method comprises the steps of:

a. employing computational means to perform a fitting operation between the chemical entity and the CnA/CnB binding pocket or the CnA/CnB homologue binding pocket; and

b. analyzing the results of said fitting operation to quantify the association between the chemical entity and the CnA/CnB binding pocket or the CnA/CnB homologue binding pocket.

22. (Amended) The method according to claim 19, wherein said crystallized molecule or molecular complex further comprises a second binding pocket defined by CnA amino acids 122, 124, 159, 160, 310, 312, 313, 314, 339, 341, 343, 344, 345, 347, 351, 352, 353, 354, 355, 356, 359, 360, and 363; and CnB amino acids 49, 50, 114, 115, 118, 119, 121, 122, 123, 124, 157, 158, 159, 161, and 162; according to

Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a second homologue binding pocket that has a root mean square deviation from the backbone atoms of said CnA and CnB amino acids of not more than 1.5Å.

23. (Amended) The method according to claim 22, wherein said molecule or molecular complex is defined by a set of structure coordinates according to Figure 1, or a homologue thereof, wherein said homologue has a root mean square deviation from the backbone atoms of said CnA and CnB amino acids of not more than 1.5Å.

24. (Amended) The method according to claim 22, wherein said molecule or molecular complex comprises amino acids 17-392 of CnA, amino acids 1-169 of CnB, amino acids 1-107 of FKBP12 and FK506.

REMARKS

In the Specification

Applicants have amended the specification at page 1 to cross-reference the present application to an earlier application from which it claims priority.